

Competition between d-wave and topological p-wave superconductivity in the doped Kitaev-Heisenberg model

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The competition between Kitaev and Heisenberg interactions away from half filling is studied for the hole-doped Kitaev-Heisenberg t - J_K - J_H model on a honeycomb lattice. While the isotropic Heisenberg coupling supports a time-reversal violating d-wave singlet state, we find that the Kitaev interaction favors a time-reversal invariant p-wave superconducting phase, which obeys the rotational symmetries of the microscopic model, and is robust for $J_H < J_K/2$. Within the p-wave superconducting phase, a critical chemical potential $|\mu| = \mu_c \approx t$ separates a topologically trivial phase for $|\mu| < \mu_c$ from a topologically non-trivial Z_2 time-reversal invariant spin-triplet phase for $|\mu| > \mu_c$.

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The concept of topological order, originally introduced in the context of quantum Hall systems, has recently been extended to topological band insulators and topological superconductors [1, 2]. One of the exciting properties of these systems is the prospect of observing non-abelian quasi-particles. A prototype model for non-abelian quasi-particles is the Kitaev model on the honeycomb lattice with a non-abelian topological phase [3].

There is both experimental [4, 5] and theoretical [6] evidence that a Kitaev model with an admixture of antiferromagnetic Heisenberg exchange is realized in iridates (Li_2IrO_3 and Na_2IrO_3) with a honeycomb lattice. For dominant Kitaev coupling, the ground state is a spin liquid. Upon increasing the relative strength of the nearest-neighbor Heisenberg coupling, the ground state first turns into a stripy antiferromagnetic phase and then into a Neel antiferromagnet [7, 8]. Both Li_2IrO_3 and Na_2IrO_3 are found to be magnetically ordered at low temperatures [4, 5, 9–11]. The temperature dependence of the magnetic susceptibility [4, 5] and the recent resonant x-ray and neutron scattering experiments [9–11] indicate that the ground state of Na_2IrO_3 is most likely described by a zig-zag spin structure. This type of magnetic order can be theoretically explained by including further neighbor Heisenberg couplings [5, 12] or in terms of trigonal distortion of the oxygen octahedra [13]. On the other hand, based on the magnetic susceptibility measurements for Li_2IrO_3 , it has been suggested that Li_2IrO_3 may be close to the Kitaev spin liquid regime [5].

The Kitaev spin model can be viewed as a Mott insulator at half filling, and one can ask about its phase diagram away from half filling. It is known that a Heisenberg antiferromagnet on the honeycomb lattice becomes a d-wave superconductor upon doping [14]. Hence one may expect superconductivity in the doped Kitaev model, and can ask how the superconducting order parameter depends on the relative strengths of antiferromagnetic Heisenberg exchange and the Kitaev interac-

tion. In this paper, we address this question by studying the Heisenberg-Kitaev model in a slave boson theory, and find that the Kitaev model turns into a p-wave superconductor upon doping, with an internal spin-orbital structure of Cooper pairs as illustrated in Fig. 1(a). When the doping level is larger than one quarter, this superconductor is an example of a time-reversal invariant Z_2 topological superconductor [15–22], which supports a pair of counter-propagating helical Majorana modes at the edges of the sample and one pair of Majorana zero modes at the vortices. This p-wave superconductor is considerably more robust to adding a Heisenberg exchange than the spin liquid phase itself at zero doping, thus raising the possibility that it might be observable in doped iridates. We also find that the time-reversal invariant topological superconductivity is not sensitive to the details of the band structure. Thus, the physics discussed here should be representative for a broad class of materials with strong spin-orbit coupling.

We consider a honeycomb lattice with three inequivalent nearest-neighbor bonds referred to as $\gamma = x, y, z$ [see Fig. 1(b)]. The Kitaev-Heisenberg model with nearest neighbor hopping is given by

$$H = -J_K \sum_{\langle ij \rangle} S_i^\gamma S_j^\gamma + J_H \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4} \right) + H_T. \quad (1)$$

The first term in the Hamiltonian (1) is called the Kitaev interaction [3], and it describes an Ising-like coupling between the γ components of spins $S_i^\gamma = \frac{1}{2} f_{i,\alpha}^\dagger \sigma_{\alpha\beta}^\gamma f_{i,\beta}$ at each bond in the γ -direction. The second term describes an isotropic Heisenberg interaction with interaction strength J_H , and H_T is the kinetic term

$$H_T = -t \sum_{\langle ij \rangle, \sigma} f_{i,\sigma}^\dagger f_{j,\sigma} + h.c. \quad (2)$$

We assume that at half-filling the system can be viewed as a Mott insulator and adopt the so-called U(1) slave

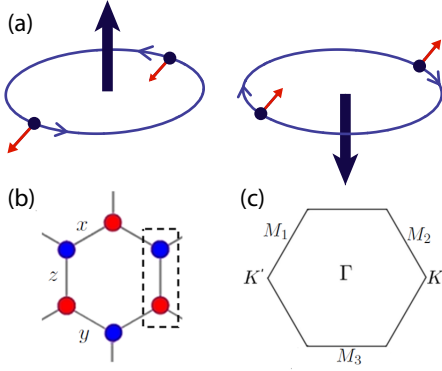


FIG. 1: (color online) (a) Relative orientations of the Cooper pair orbital (thick arrows) and spin (thin red arrows) angular momentum in the ground state wave function for topologically nontrivial time-reversal invariant p -wave pairing. Conventions for (b) real space and (c) reciprocal lattices. The four time reversal invariant points in the Brillouin zone are Γ , M_1 , M_2 , and M_3 .

boson method to take into account the renormalization of the hopping amplitude by strong correlations [23, 24]. By assuming that the holons are condensed to give a coherent Fermi-liquid state, the hopping amplitude t can be written as $t = t_0\delta$, where t_0 is the bare matrix element and δ quantifies the hole doping so that $1 - \delta$ is the average number of electrons per site.

We introduce a spin-singlet and three spin-triplet operators, defined respectively as $s_{ij} = (f_{i\uparrow}f_{j\downarrow} - f_{i\downarrow}f_{j\uparrow})/\sqrt{2}$, $t_{ij,x} = (f_{i\downarrow}f_{j\downarrow} - f_{i\uparrow}f_{j\uparrow})/\sqrt{2}$, $t_{ij,y} = i(f_{i\downarrow}f_{j\downarrow} + f_{i\uparrow}f_{j\uparrow})/\sqrt{2}$, $t_{ij,z} = i(f_{i\uparrow}f_{j\downarrow} + f_{i\downarrow}f_{j\uparrow})/\sqrt{2}$, and re-write the Kitaev-Heisenberg part of the Hamiltonian in terms of these operators. The Kitaev term on an x -link is given by

$$-S_i^x S_j^x = \frac{1}{4} [s_{ij}^\dagger s_{ij} + t_{ij,x}^\dagger t_{ij,x} - t_{ij,y}^\dagger t_{ij,y} - t_{ij,z}^\dagger t_{ij,z}], \quad (3)$$

and for y - and z -links the plus sign appears in front of the $t_{ij,y}^\dagger t_{ij,y}$ and $t_{ij,z}^\dagger t_{ij,z}$ operators, respectively.

The mean field Hamiltonian is obtained by replacing the spin-singlet and spin-triplet operators by their expectation values in the usual fashion. We denote the spin-singlet and spin-triplet expectation values by Δ_γ and d_γ^ρ respectively, where γ corresponds to the bond direction, and ρ the component of the mean-field triplet vector, such that

$$\begin{aligned} \Delta_\gamma &= -\frac{1}{\sqrt{2}} \left(J_H - \frac{J_K}{4} \right) \langle s_{ij} \rangle \quad \text{for } \gamma \text{ bonds,} \\ d_\gamma^\rho &= \frac{J_K}{4\sqrt{2}} \langle t_{ij,\rho} \rangle \quad \text{for } \gamma \text{ bonds.} \end{aligned} \quad (4)$$

A different decoupling of the Kitaev interaction into both hopping and pairing channels was used in [25] to describe the undoped Kitaev model. Here we consider only the pairing channel, which is justified in the limit of reasonably large doping.

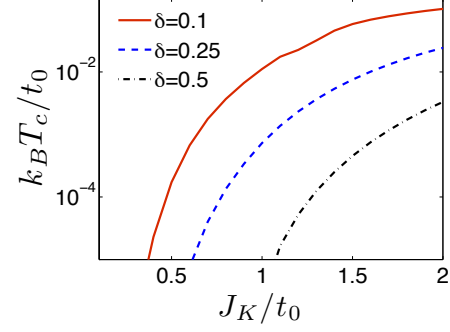


FIG. 2: (color online) The transition temperature $k_B T_c / t_0$ in the p -wave triplet channel as a function of the Kitaev interaction strength J_K / t_0 for different doping levels $\delta = 0.1, 0.25, 0.5$, at $J_H = 0$ [30].

At the critical temperature for the superconducting phase transition the order parameter vanishes and we obtain linearized gap equations [26]. The spin singlet case was previously solved in Ref. 14, obtaining a mixed superconducting phase of d -wave intraband pairing and p -wave interband pairing. Following a similar procedure we obtain linearized gap equations also for the spin-triplet order parameters. We find that the d_γ^ρ with different ρ are not coupled in these equations and therefore we can conveniently write the linearized gap equations for triplet order parameters using three stability matrices $M_{x,y,z}$. The critical temperatures for the different channels can be obtained by finding the largest temperature where at least one of the eigenvalues of the stability matrix is equal to 1. The possible solutions of the order parameter near the critical temperature are linear combinations of the eigenvectors corresponding to this eigenvalue.

We find that the stability matrix for d_γ^x is

$$M_x = \frac{J_K}{4} \begin{pmatrix} -B & C & C \\ -C & B & C \\ -C & C & B \end{pmatrix}. \quad (5)$$

The stability matrices M_y and M_z can be obtained from M_x by cyclically changing the column of negative signs. The matrix elements are $B = A_{i=j}$ and $C = A_{i \neq j}$, where

$$\begin{aligned} A_{ij} = \frac{1}{2N} \sum_{\vec{q}} & \left[\left(\frac{\tanh(\beta_c \xi_1/2)}{2\xi_1} + \frac{\tanh(\beta_c \xi_2/2)}{2\xi_2} \right) \right. \\ & \cdot \sin(\vec{\delta}_i \cdot \vec{q} - \phi) \sin(\vec{\delta}_j \cdot \vec{q} - \phi) \\ & \left. + \frac{\sinh(\beta_c \mu) \cos(\vec{\delta}_i \cdot \vec{q} - \phi) \cos(\vec{\delta}_j \cdot \vec{q} - \phi)}{2\mu \cosh(\beta_c \xi_1/2) \cosh(\beta_c \xi_2/2)} \right], \end{aligned} \quad (6)$$

in which $\beta_c = 1/(k_B T_c)$, $\vec{\delta}_i$ denote the nearest neighbor vectors, $\xi_{1(2)} = \pm |t(\vec{q})| - \mu$ are the single particle dispersions, $t(\vec{q}) = t \sum_j e^{i\vec{\delta}_j \cdot \vec{q}}$ and $\phi = \arg[t(\vec{q})]$.

Because of the symmetry relation of the matrices $M_{x,y,z}$, the eigenvectors of the linearized gap

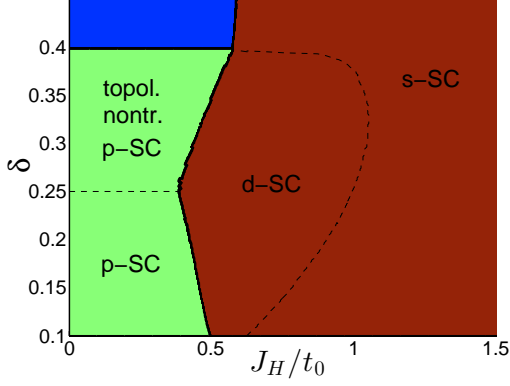


FIG. 3: (color online) Phase diagram for the condensation in the spin-singlet (red/dark gray regions marked as s-SC and d-SC) and spin-triplet (green/light gray regions) channels as a function of Heisenberg interaction J_H and doping δ , for Kitaev interaction strength $J_K = t_0$. In the singlet channel both d-wave and s-wave order parameters can exist depending on the doping and interaction strength. The d-wave order parameter breaks the time-reversal symmetry. Within the p-wave triplet phase, there is a topological phase transition (indicated by dashed line) between topologically trivial $\delta < 0.25$ and topologically non-trivial $\delta > 0.25$ time-reversal invariant superconducting states. The (blue/dark gray) region in the upper left corner of the phase-diagram denotes the parameter regime where $k_B T_c < 10^{-4} t_0$.

equation with largest critical temperature are three-fold degenerate. By denoting the solutions as $\mathbf{d} = (d_x^x, d_y^x, d_z^x, d_x^y, d_y^y, d_z^y, d_x^z, d_y^z, d_z^z)$, the linearly independent solutions are

$$\begin{aligned} \mathbf{d}_1 &= (0, -1, 1, 0, 0, 0, 0, 0, 0), \\ \mathbf{d}_2 &= (0, 0, 0, 1, 0, -1, 0, 0, 0), \\ \mathbf{d}_3 &= (0, 0, 0, 0, 0, 0, -1, 1, 0). \end{aligned} \quad (7)$$

We now compare the critical temperatures for superconducting condensation in the spin-singlet and spin-triplet channels. In Fig. 2 we show the critical temperatures for the onset of spin-triplet superconductivity at various doping levels. In the spin-singlet channel, the Kitaev interaction affects the pairing only by renormalizing the interaction strength J_H and therefore the critical temperatures for singlet-superconductivity can be obtained using the theory of Ref. 14 that predicts a time-reversal violating d-wave state (analogous to that found for a doped Heisenberg model in a triangular lattice [27–29]) or s-wave state depending on the interaction strength and doping. The phase diagram is shown in Fig. 3, where the dominant condensation channel is computed as a function of doping and Heisenberg interaction J_H for fixed Kitaev interaction strength $J_K = t_0$. Interestingly, we find that the phase transition between triplet and singlet superconductivity appears at the relative interaction strength $J_H/J_K \simeq 1/2$. We note that in the absence of doping the topologically interesting Kitaev spin

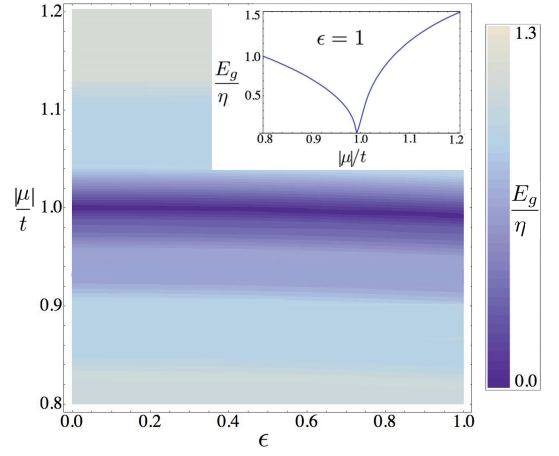


FIG. 4: (color online) The minimum energy required to excite quasiparticles as a function of the dimensionless interband order parameter strength ϵ and chemical potential $|\mu|$ for $\eta = 0.042t$. The interband order parameter is adiabatically switched on when ϵ changes from $\epsilon = 0$ to $\epsilon = 1$. The inset demonstrates that for each value of ϵ the energy gap closes in the vicinity of $|\mu| = t$ indicating a transition between the topologically trivial and nontrivial states.

liquid phase exists only in the range $J_H < J_K/8$ [7, 8]. This indicates that the spin-triplet superconductivity is very robust to the presence of the Heisenberg interaction, and therefore might be observable in doped iridates.

The order parameter for triplet superconductivity at temperatures below the T_c can now be calculated from the nonlinear gap equations. We assume that the order parameter is a linear combination of the three degenerate solutions to the linearized gap equations, and so we can write $\mathbf{d} = (\eta_1 \mathbf{d}_1 + \eta_2 \mathbf{d}_2 + \eta_3 \mathbf{d}_3)$. Solving the gap equations iteratively from different initial conditions, we find four solutions $(\eta_1, \eta_2, \eta_3) = \eta(1, \pm 1, \pm i)$. These solutions have large basins of attraction. Moreover, the real parts of the eigenvalues of the stability matrices obtained by linearizing the gap equation around these solutions are smaller than one, indicating stability. Within our mean field approach, the magnitude of η depends on temperature, doping, and the interaction strength J_K [30]. For $k_B T = 10^{-4} t$, $|\mu| = 1.2t$ (corresponding to $\delta \approx 0.38$) and $J_K = 2.3t_0$, we obtain $\eta \approx 0.042t$. This value of η is used for Figs. 4 and 5.

By expressing the intra- and interband order parameters using the convention $i(\mathbf{d}(\vec{q}) \cdot \vec{\sigma})\sigma_2$ [26], we obtain expressions for the intra- and interband \mathbf{d} -vectors in momentum space. Expanding these solutions around the Γ point, we obtain

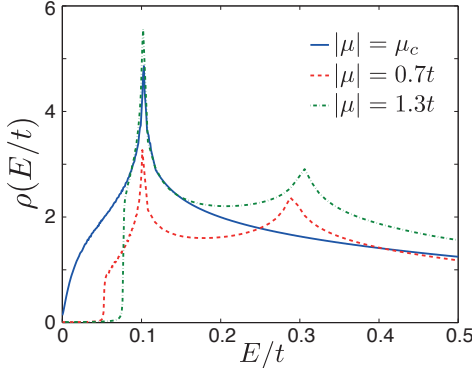


FIG. 5: (color online) Integrated density of states for $\eta = 0.042t$ and chemical potentials $0.7t$, μ_c , and $1.3t$. The critical value of the chemical potential is $\mu_c = 0.9932t$.

$$\begin{aligned} \mathbf{d}_{11}(\vec{q}) &= i\eta \left(-\frac{q_x}{2} + \frac{\sqrt{3}q_y}{2}, \pm \left(\frac{q_x}{2} + \frac{\sqrt{3}q_y}{2} \right), \pm q_x \right), \\ \mathbf{d}_{12}(\vec{q}) &= \frac{\eta}{24} \left(-3q_x^2 + 2\sqrt{3}q_xq_y + 3q_y^2, \right. \\ &\quad \left. \pm (-3q_x^2 - 2\sqrt{3}q_xq_y + 3q_y^2), \mp 4\sqrt{3}q_xq_y \right), \end{aligned} \quad (8)$$

where $\mathbf{d}_{22} = -\mathbf{d}_{11}$ are the intraband pairing vectors, and $\mathbf{d}_{21} = -\mathbf{d}_{12}$ are the interband pairing vectors. Using these $\mathbf{d}_{ij}(\vec{q})$ -vectors we find that the numerical solution of the nonlinear gap equations is that of a *time-reversal symmetric odd parity* phase in the dominant intraband channel, and a *time-reversal symmetric even parity* phase in the interband channel. Both order parameters retain the six-fold rotational symmetry of the lattice, and so the phases obtained obey all the underlying symmetries of the microscopic model [31].

The order parameter \mathbf{d}_{11} in Eq. (8) lies on a circle with fixed $|\mathbf{d}_{11}|$ when \vec{q} rotates around a circle in the (q_x, q_y) -plane. The axis \mathbf{r}_d around which \mathbf{d}_{11} rotates depends on the choice of signs in Eq. (8). For example, the choice $(-, +)$ corresponds to a rotation axis along the $(1, 1, 1)$ direction. By virtue of a global transformation of the spin quantization axis in the model Eq. (1), the \mathbf{d}_{11} vector is rotated into the xy -plane, and describes a $q_x - iq_y$ pairing for spin-up and a $q_x + iq_y$ pairing for spin-down (equivalent to the B-phase of superfluid ^3He) components of the order parameter. In the original model Eq. (1), this corresponds to $q_x - iq_y$ pairing for spins pointing in the $(1, 1, 1)$ direction and $q_x + iq_y$ pairing for spins pointing in the $(-1, -1, -1)$ direction, see Fig. 1(a).

In the absence of interband coupling and in the weak pairing limit, the value of the Z_2 invariant of a time-reversal invariant topological superconductor is determined by the topology of the Fermi surface [18–22]. More precisely, its value is determined by the parity of the number of time-reversal invariant points below the Fermi

level. On the honeycomb lattice, the Fermi surface topology changes from hole pockets around the two inequivalent K points to a particle-like Fermi surface around the Γ point when the chemical potential is tuned through the critical value $|\mu| = \mu_c = t$ (corresponding to the critical value of hole doping $\delta_c = 0.25$). For $|\mu| < \mu_c$, there are four time-reversal invariant points below the Fermi level (the three M points and the Γ point shown in Fig. 1), and the superconductor is in a topologically trivial phase. At the special point $|\mu| = \mu_c$ in the single particle dispersion, the Fermi surface touches the three inequivalent time-reversal symmetric M points. As a consequence, for $|\mu| > \mu_c$, the only time-reversal invariant point enclosed by the Fermi surface is the Γ point. Because the intraband order parameter has odd parity, the superconductor in the absence of interband order parameter is guaranteed to be a topologically non-trivial superconductor [18–22], in the class DIII [15]. Adiabatically switching on the interband pairing, we find that the quasiparticle dispersion indeed remains gapped in each topological regime and that the value of the critical chemical potential μ_c , where the quasiparticle dispersion becomes gapless, is renormalized downwards. Therefore, the topological phase transition remains robust in the presence of the even parity interband phase (see Fig. 4). This phase transition is shown with a dashed line in Fig. 3.

The topological phase transition can be observed by measuring the density of states as a function of energy, e.g., by NMR and tunneling experiments. Fig. 5 shows the density of states as a function of energy for three different values of chemical potential. Above and below $|\mu| = \mu_c$ the density of states vanishes at low energies resulting in an energy gap, which is of the order of η . On the other hand, at the phase transition $|\mu| = \mu_c$ the energy gap closes resulting in an increased density of states at low energies.

A few remarks are in order concerning the relevance of our results for the actual materials. First, we have considered here the nearest-neighbor hopping Hamiltonian, but our results are in fact robust with respect to changes in the band structure. We have verified that all our qualitative results remain valid if a second nearest neighbor hopping $t' = 0.1t$ is introduced. Second, the necessary values of the Kitaev interaction strength for the existence of topological p-wave superconductivity might seem quite large $J_K > 0.7t_0$. Nevertheless, these values are not unrealistic for the iridates, because the relation between the exchange interaction strength and the effective nearest-neighbor hopping in iridates is not as simple as, for example, in cuprates. In systems with strong spin-orbit coupling, the electron collects a phase factor during the superexchange process giving rise to a Kitaev interaction, and, at the same time, the effective nearest-neighbor hopping amplitude is strongly reduced by negative quantum interference. We also notice that approximately similar values of the exchange interaction

strength have been discussed for graphene [14].

In summary, we have studied the competition of spin-singlet d-wave superconductivity and spin-triplet p-wave superconductivity in the hole-doped Kitaev-Heisenberg model on a honeycomb lattice. We have shown that the Kitaev interaction favors a time-reversal invariant Z_2 topological superconductivity, which is robust to the presence of an isotropic Heisenberg interaction $J_H < J_K/2$. Because this topological phase supporting pairs of counter-propagating Majorana modes persists over a much wider region of the phase diagram than the Kitaev spin liquid phase itself in the absence of doping, it might be easier to find materials where it becomes observable.

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 - [30] Within the present mean field approach, J_H below its critical value does not affect T_c and the amplitude of the order parameter in the triplet channel, but fluctuation corrections from J_H may reduce them.
 - [31] After completion of this work, we have become aware of the preprint by Y. You, I. Kimchi, and A. Vishwanath, arXiv:1109.4155, where a doped Kitaev-Heisenberg model is studied using the SU(2) slave boson representation. You *et al.* also find a p-wave spin-triplet state; however, their order parameter breaks time-reversal symmetry in contrast to our result. While we found that the time-reversal violating state is slightly higher in energy, it remains to be clarified whether correlation effects beyond the present level of approximations would tip a balance between the two solutions.